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HPCS Application Analysis and Assessment

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Abstract

The value of a HPC system to a user includes many factors, such as: execution time on a particular problem, software development time, and both direct and indirect costs. The DARPA High Productivity Computing Systems is focused on providing a new generation of economically viable high productivity computing systems for the national security and industrial user community in the 2007-2010 timeframe. The goal is to provide systems that double in productivity (or value) every 18 months. This program has initiated a fundamental reassessment of how we define and measure performance, programmability, portability, robustness and ultimately productivity in the HPC domain. This talk will describe the HPCS efforts to develop a productivity assessment framework (see Figure 1), characterize HPC user workflows, and define the scope of the target applications.

Introduction

The HPCS program seeks to create trans-Pefaflop systems of significant value to the Government HPC community. Such value will be determined by assessing many additional factors beyond just theoretical peak flops (i.e. "Machoflops"). Ultimately, the goal is to decrease the time-to-solution, which means decreasing both the execution time and development time of an application on a particular system. Evaluating the capabilities of a system with respect to these goals requires a different assessment process. The goal of the HPCS assessment activity is to prototype and baseline a process that can be transitioned to the acquisition community for 2010 procurements.

Development Time

The most novel part of the assessment activity will be the effort to measure/predict the ease or difficulty of developing HPC applications. Currently, there is no quantitative methodology for comparing the development time impact of various HPC programming technologies. To achieve this goal, we will use a variety of tools including

- Application of code metrics on existing HPC codes
- Several prototype analytic models of development time
- Interface characterization (e.g. language, parallel model, memory model, …)
- Scalable benchmarks designed for testing both performance and programmability
- Classroom software engineering experiments
- Human validated demonstrations

These tools will provide the baseline data necessary for modeling development time and allow the new technologies developed under HPCS to be assessed quantitatively.

This work is sponsored by Defense Advanced Research Projects Administration, under Air Force Contract F19628-00-C-0002. Opinions, interpretations, conclusions and recommendations are those of the author and are not necessarily endorsed by the United States Government.

Report Documentation Page

Form Approved
OMB No. 0704-0188

1. REPORT DATE **23 SEP 2003**	2. REPORT TYPE **N/A**	3. DATES COVERED **-**

4. TITLE AND SUBTITLE **HPCS Application Analysis and Assessment**	5a. CONTRACT NUMBER 5b. GRANT NUMBER 5c. PROGRAM ELEMENT NUMBER
6. AUTHOR(S)	5d. PROJECT NUMBER 5e. TASK NUMBER 5f. WORK UNIT NUMBER
7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES) **MIT Lincoln Laboratory; The MITRE Corporation**	8. PERFORMING ORGANIZATION REPORT NUMBER
9. SPONSORING/MONITORING AGENCY NAME(S) AND ADDRESS(ES)	10. SPONSOR/MONITOR’S ACRONYM(S) 11. SPONSOR/MONITOR’S REPORT NUMBER(S)

12. DISTRIBUTION/AVAILABILITY STATEMENT

Approved for public release, distribution unlimited

13. SUPPLEMENTARY NOTES

See also ADM001694, HPEC-6-Vol 1 ESC-TR-2003-081; High Performance Embedded Computing (HPEC) Workshop(7th). , The original document contains color images.

14. ABSTRACT

15. SUBJECT TERMS

16. SECURITY CLASSIFICATION OF:			17. LIMITATION OF ABSTRACT	18. NUMBER OF PAGES	19a. NAME OF RESPONSIBLE PERSON
a. REPORT **unclassified**	b. ABSTRACT **unclassified**	c. THIS PAGE **unclassified**	**UU**	**35**	

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Execution Time
The execution time part of the assessment activity will leverage the strong heritage in the HPC performance modeling community. This will include analytic, source code, and executable based tools for analyzing the projected performance of various applications on current, next generation and HPCS designs. The execution time and development time activities will be strongly coupled so as to provide a clear picture to the community of the tradeoffs that exist between execution time and development time.

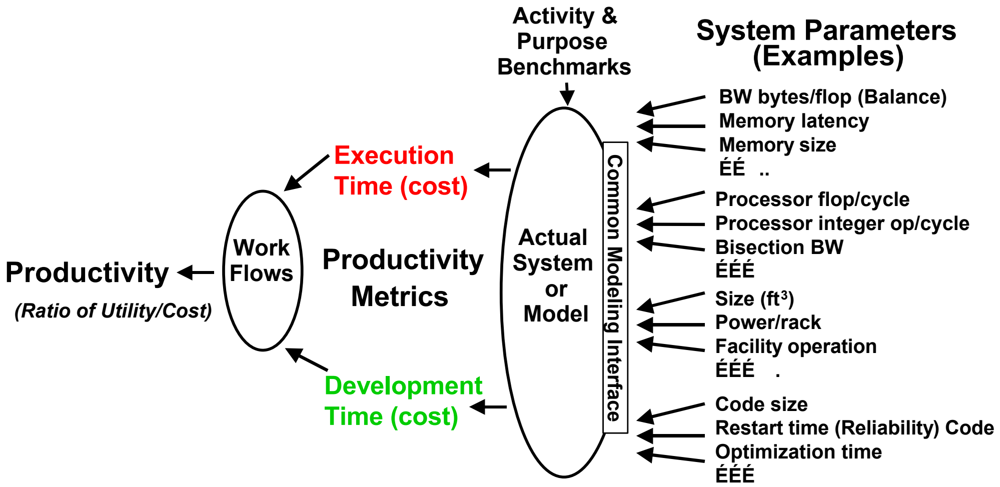

Figure 1: HPCS Assessment Framework. The goal of the framework is to provide a mechanism for integrating system specific capabilities with user specific needs to assess the value of a particular machine for a particular mission.

HPCS Application Analysis and Assessment

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Dr. David Koester / MITRE

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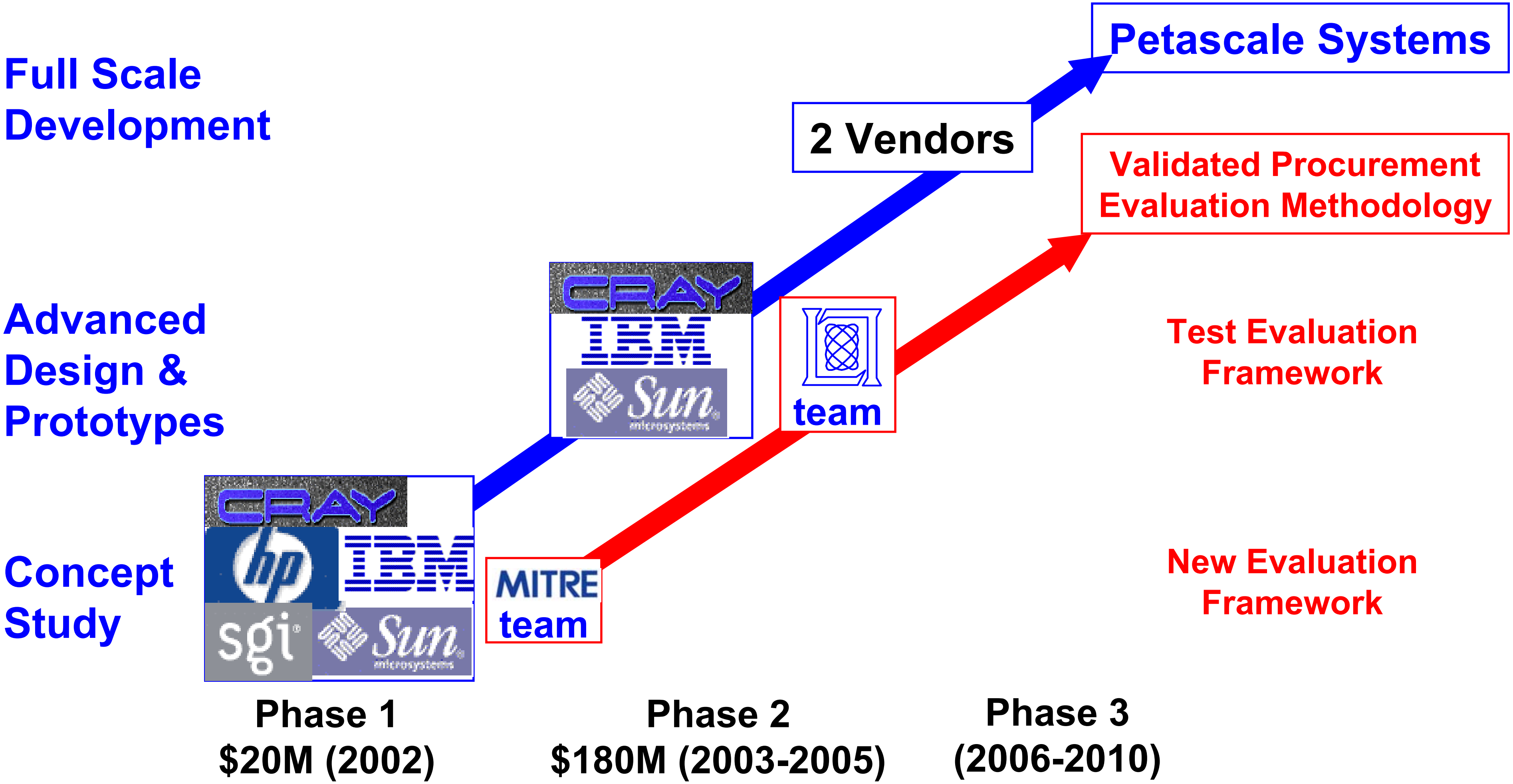
Outline

- **Introduction**
  - *Motivation*
  - *Productivity Framework*
- Workflows
- Metrics
- Models & Benchmarks
- Schedule and Summary

High Productivity Computing Systems
-Program Overview-

- Create a new generation of economically viable computing systems and a procurement methodology for the security/industrial community (2007 – 2010)



Full Scale Development

Advanced Design & Prototypes

Concept Study

Petascale Systems

2 Vendors

Validated Procurement Evaluation Methodology

Test Evaluation Framework

New Evaluation Framework

Phase 1
$20M (2002)

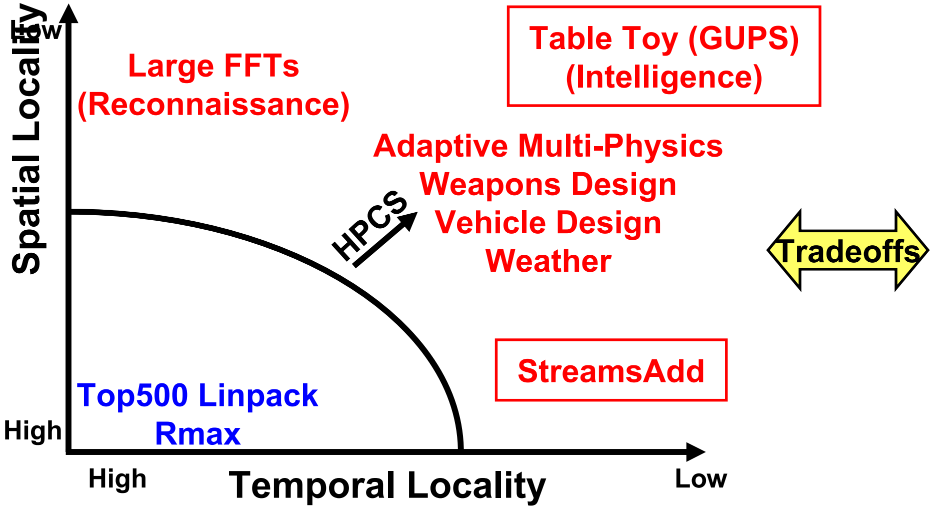
Phase 2
$180M (2003-2005)

Phase 3
(2006-2010)

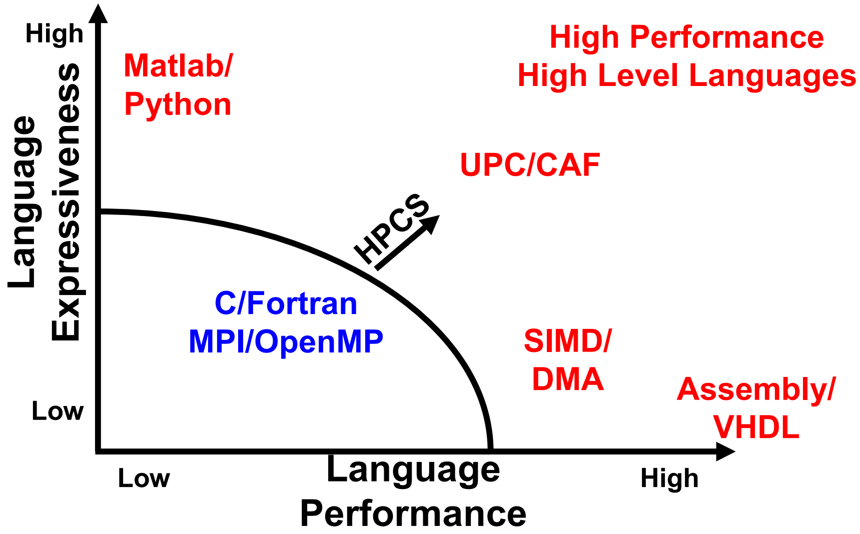
Motivation: Metrics Drive Designs

"You get what you measure"

Execution Time (Example)



Development Time (Example)



Current metrics favor caches and pipelines

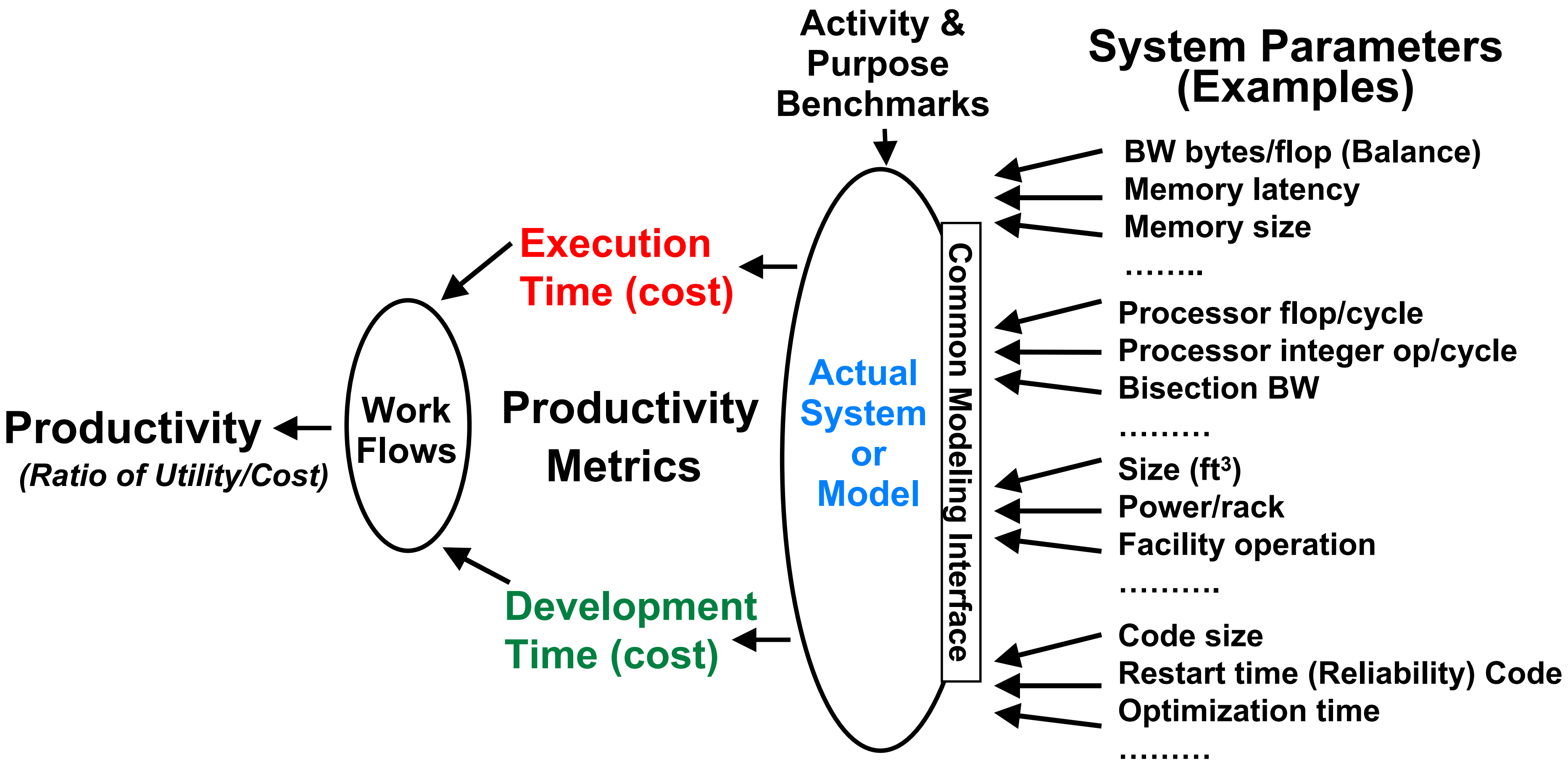
- Systems ill-suited to applications with
- Low spatial locality
- Low temporal locality

No metrics widely used

- Least common denominator standards
- Difficult to use
- Difficult to optimize

- HPCS needs a validated assessment methodology that values the "right" vendor innovations
- Allow tradeoffs between Execution and Development Time

Phase 1: Productivity Framework



Activity & Purpose Benchmarks

System Parameters (Examples)

- BW bytes/flop (Balance)
- Memory latency
- Memory size
- ……..
- Processor flop/cycle
- Processor integer op/cycle
- Bisection BW
- ………
- Size (ft^3)
- Power/rack
- Facility operation
- ……….
- Code size
- Restart time (Reliability) Code
- Optimization time
- ………

Common Modeling Interface

Actual System or Model

Execution Time (cost)

Development Time (cost)

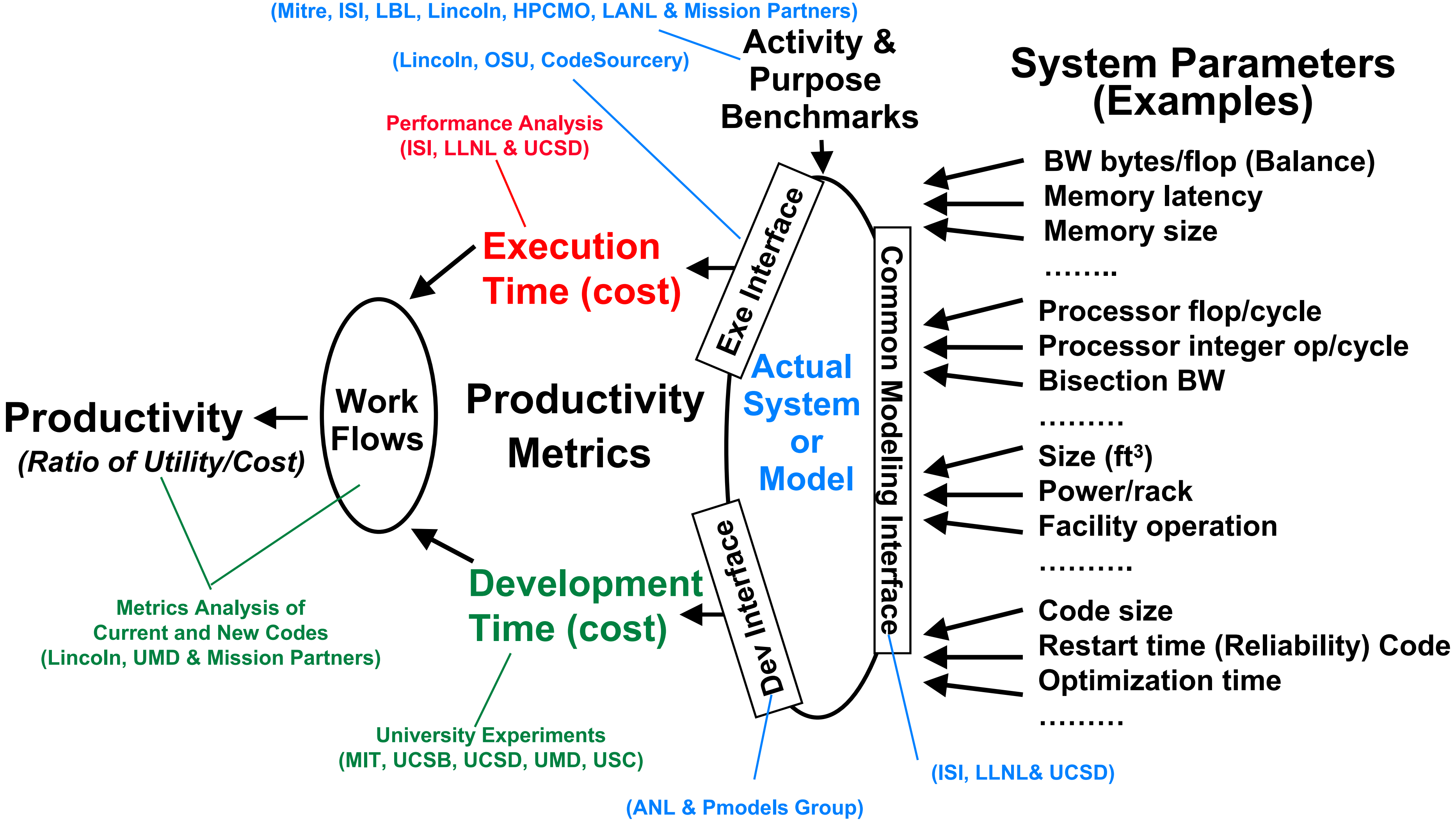
Productivity Metrics

Work Flows

Productivity

(Ratio of Utility/Cost)

Phase 2: Implementation



(Mitre, ISI, LBL, Lincoln, HPCMO, LANL & Mission Partners)

Activity & Purpose Benchmarks

(Lincoln, OSU, CodeSourcery)

Performance Analysis (ISI, LLNL & UCSD)

Execution Time (cost)

Exe Interface

Productivity (Ratio of Utility/Cost)

Work Flows

Productivity Metrics

Actual System or Model

Common Modeling Interface

Development Time (cost)

Dev Interface

Metrics Analysis of Current and New Codes (Lincoln, UMD & Mission Partners)

University Experiments (MIT, UCSB, UCSD, UMD, USC)

(ANL & Pmodels Group)

(ISI, LLNL& UCSD)

System Parameters (Examples)

- BW bytes/flop (Balance)
- Memory latency
- Memory size
- ……..
- Processor flop/cycle
- Processor integer op/cycle
- Bisection BW
- ………
- Size (ft^3)
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- ……….
- Code size
- Restart time (Reliability) Code
- Optimization time
- ………

Outline

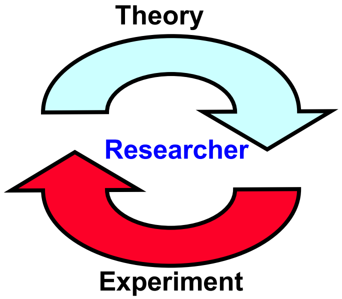
- Introduction
- **Workflows**
  - *Lone Researcher*
  - *Enterprise*
  - *Production*
- Metrics
- Models & Benchmarks
- Schedule and Summary

HPCS Mission Work Flows

Overall Cycle

Development Cycle

Researcher

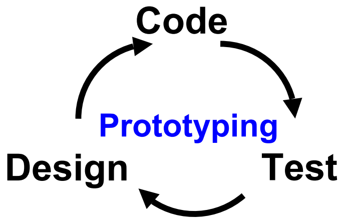


🟦 Development

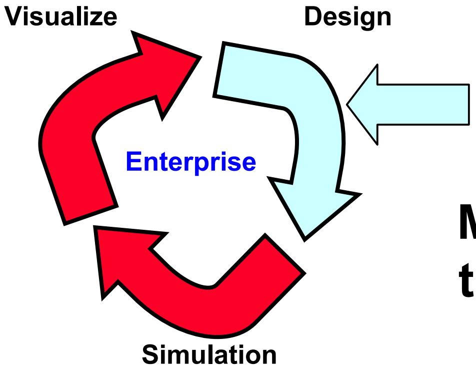
🟥 Execution

Days to hours

Hours to minutes



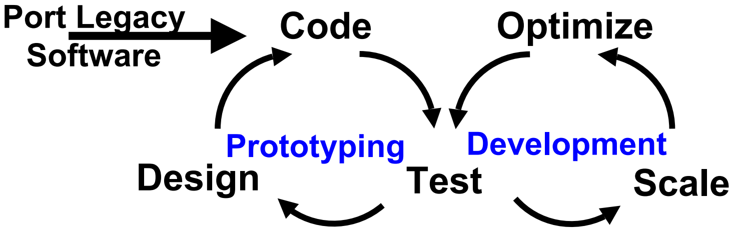
Enterprise



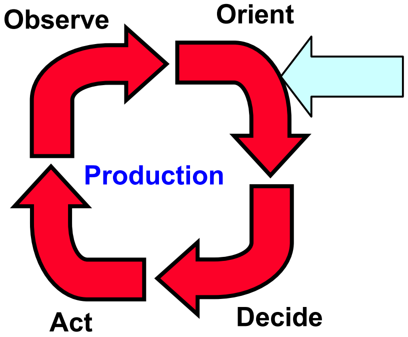
Port Legacy Software

Months to days

Months to days



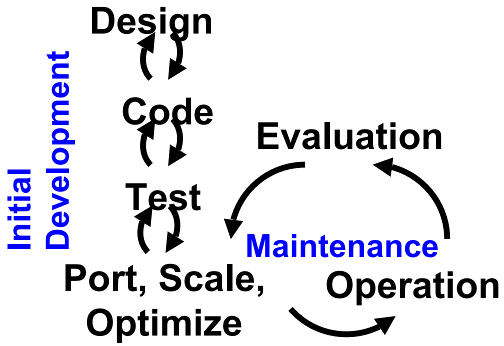
Production



Initial Product Development

Hours to Minutes (Response Time)

Years to months



HPCS Productivity Factors: Performance, Programmability, Portability, and Robustness are very closely coupled with each work flow

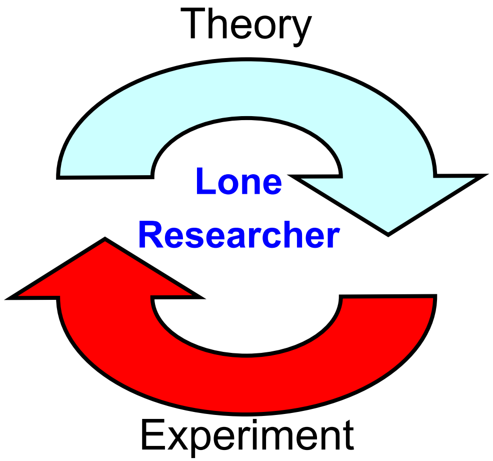
Lone Researcher

- Missions (development): Cryptanalysis, Signal Processing, Weather, Electromagnetics

- Process Overview
  - Goal: solve a compute intensive domain problem: crack a code, incorporate new physics, refine a simulation, detect a target
  - Starting point: inherited software framework (~3,000 lines)
  - Modify framework to incorporate new data (~10% of code base)
  - Make algorithmic changes (~10% of code base); Test on data; Iterate
  - Progressively increase problem size until success
  - Deliver: code, test data, algorithm specification

- Environment overview
  - Duration: months Team size: 1
  - Machines: workstations (some clusters), HPC decreasing
  - Languages: FORTRAN, C → Matlab, Python
  - Libraries: math (external) and domain (internal)

- Software productivity challenges
  - Focus on rapid iteration cycle
  - Frameworks/libraries often serial



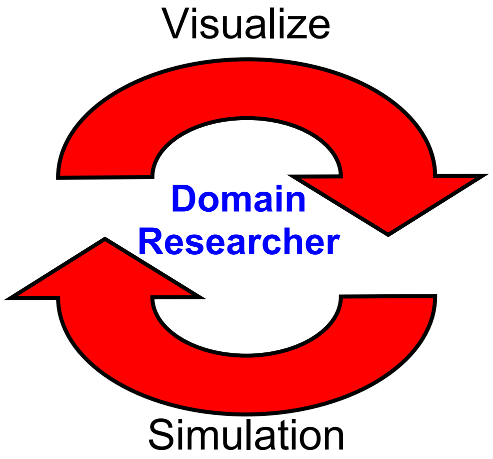
Domain Researcher (special case)

- Scientific Research: DoD HPCMP Challenge Problems, NNSA/ASCI Milestone Simulations

- Process Overview
  - Goal: Use HPC to perform Domain Research
  - Starting point: Running code, possibly from an Independent Software Vendor (ISV)
  - NO modifications to codes
  - Repeatedly run the application with user defined optimization

- Environment overview
  - Duration: months Team size: 1-5
  - Machines: workstations (some clusters), HPC
  - Languages: FORTRAN, C
  - Libraries: math (external) and domain (internal)

- Software productivity challenges — None!
- Productivity challenges
  - Robustness (reliability)
  - Performance
  - Resource center operability



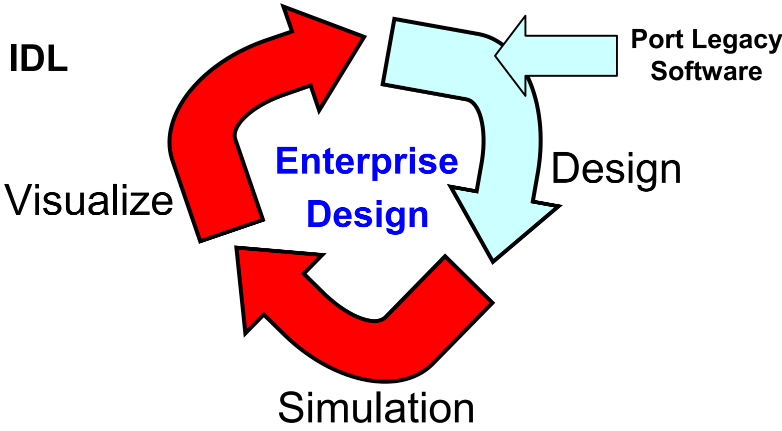
Enterprise Design

- Missions (development): Weapons Simulation, Image Processing

- Process Overview
  - Goal: develop or enhance a system for solving a compute intensive domain problem: incorporate new physics, process a new surveillance sensor
  - Starting point: software framework (~100,000 lines) or module (~10,000 lines)
  - Define sub-scale problem for initial testing and development
  - Make algorithmic changes (~10% of code base); Test on data; Iterate
  - Progressively increase problem size until success
  - Deliver: code, test data, algorithm specification, iterate with user

- Environment overview
  - Duration: ~1 year Team size: 2-20
  - Machines: workstations, clusters, hpc
  - Languages: FORTRAN, C, → C++, Matlab, Python, IDL
  - Libraries: open math and communication libraries

- Software productivity challenges
  - Legacy portability essential
    - Avoid machine specific optimizations (SIMD, DMA, …)
  - Later must convert high level language code



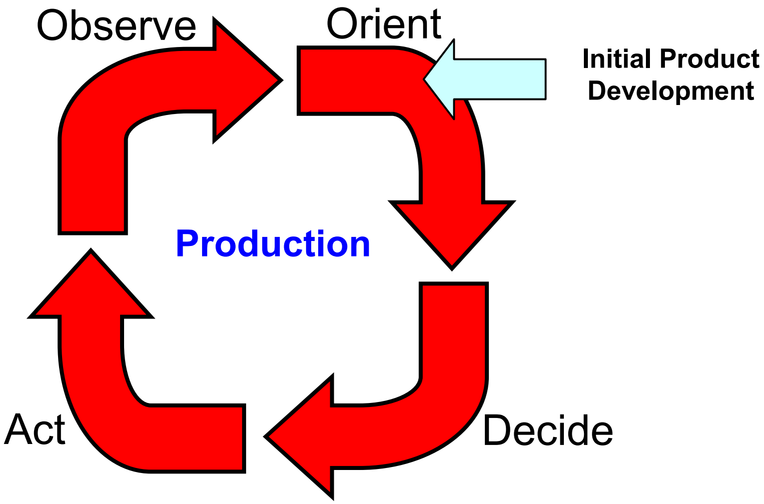
Production

- Missions (production): Cryptanalysis, Sensor Processing, Weather

- Process Overview
  - Goal: develop a system for fielded deployment on an HPC system
  - Starting point: algorithm specification, test code, test data, development software framework
  - Rewrite test code into development framework; Test on data; Iterate
  - Port to HPC; Scale; Optimize (incorporate machine specific features)
  - Progressively increase problem size until success
  - Deliver: system

- Environment overview
  - Duration: ~1 year Team size: 2-20
  - Machines: workstations and HPC target
  - Languages: FORTRAN, C, → C++

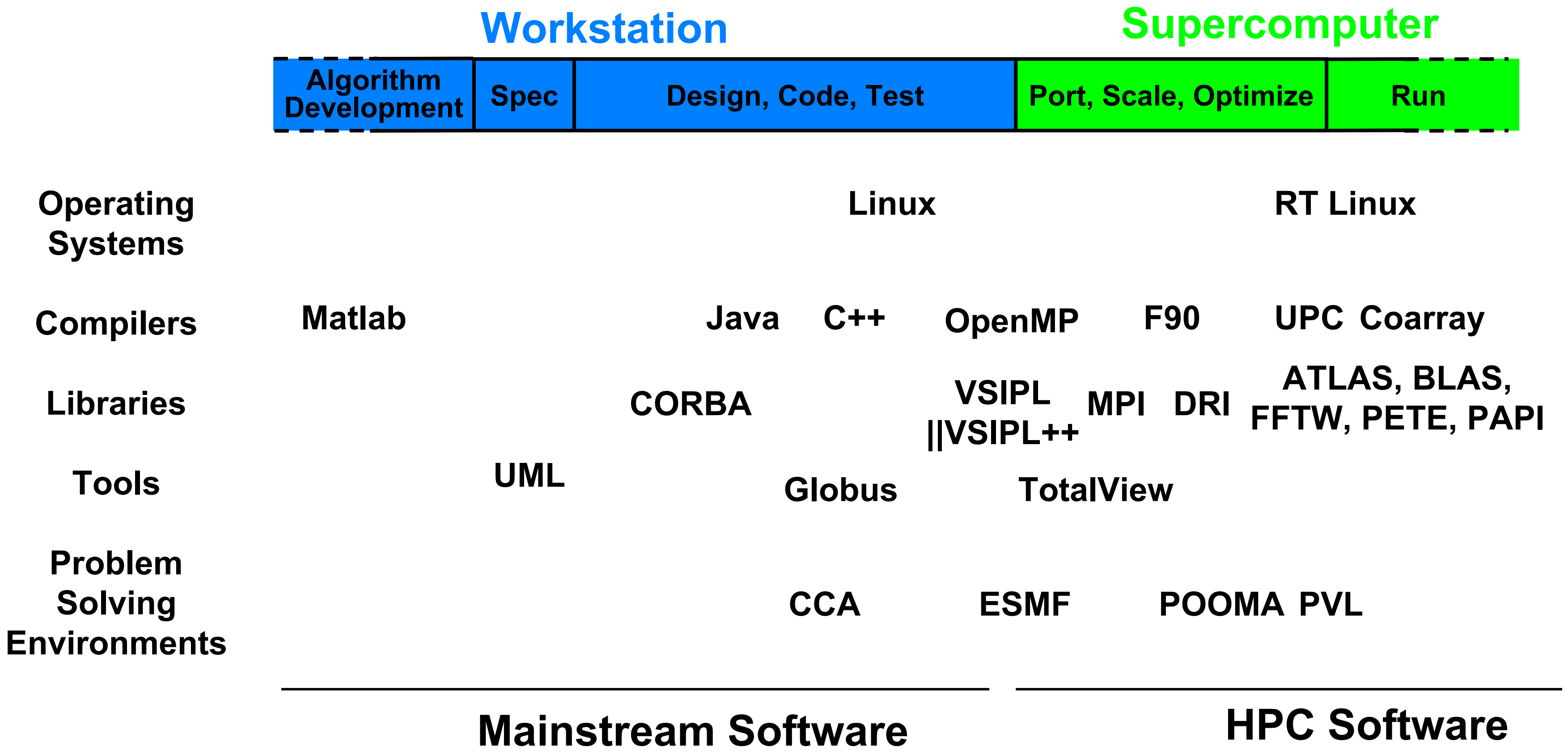
- Software productivity challenges
  - Conversion of higher level languages
  - Parallelization of serial library functions
  - Parallelization of algorithm
  - Sizing of HPC target machine



HPC Workflow SW Technologies

Production Workflow

- Many technologies targeting specific pieces of workflow
- Need to quantify workflows (stages and % time spent)
- Need to measure technology impact on stages



Workstation

Supercomputer

Algorithm Development | Spec | Design, Code, Test | Port, Scale, Optimize | Run

Operating Systems: Linux, RT Linux

Compilers: Matlab, Java, C++, OpenMP, F90, UPC, Coarray

Libraries: CORBA, VSIPL, ||VSIPL++, MPI, DRI, ATLAS, BLAS, FFTW, PETE, PAPI

Tools: UML, Globus, TotalView

Problem Solving Environments: CCA, ESMF, POOMA, PVL

Mainstream Software

HPC Software

Example: Coding vs. Testing

Workflow Breakdown (NASA SEL)

	Analysis and Design	Coding and Auditing	Checkout and Test
Sage	39%	14%	47%
NTDS	30	20	50
Gemini	36	17	47
Saturn V	32	24	44
OS/360	33	17	50
TRW Survey	46	20	34

Testing Techniques (UMD)

Code Reading

Reading by Stepwise Abstraction

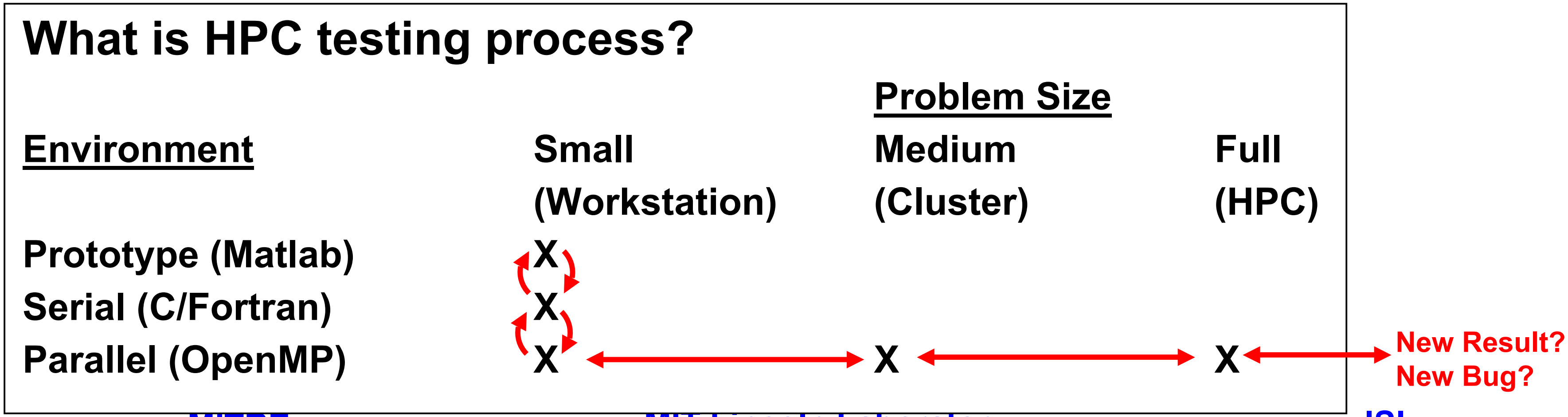
Functional Testing

Boundary Value Equivalence Partition Testing

Structural Testing

Achieving 100% statement coverage

What is HPC testing process?



		Problem Size	
Environment	Small (Workstation)	Medium (Cluster)	Full (HPC)
Prototype (Matlab)	X		
Serial (C/Fortran)	X		
Parallel (OpenMP)	X	X	X

New Result?
New Bug?

Outline

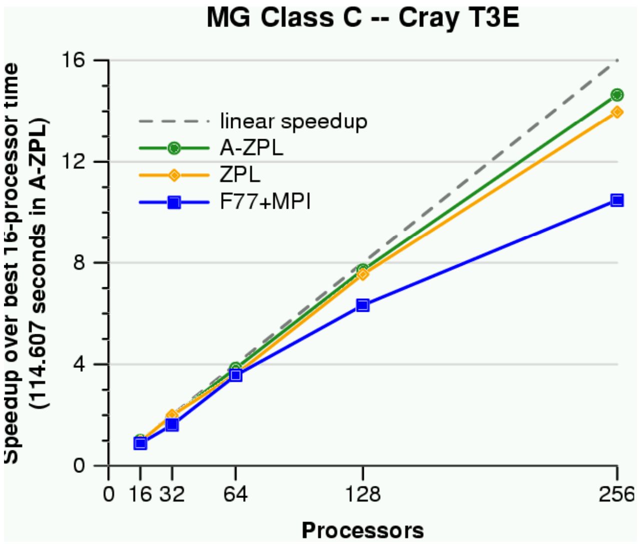
- Introduction
- Workflows
- **Metrics**
- Models & Benchmarks
- Schedule and Summary

- ***Existing Metrics***
- ***Dev. Time Experiments***
- ***Novel Metrics***

Example Existing Code Analysis

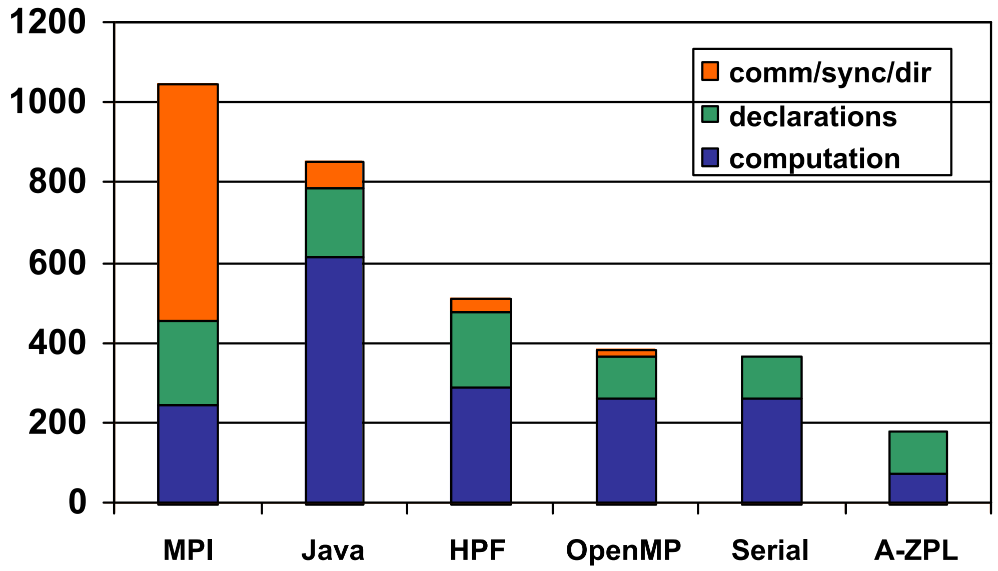
Analysis of existing codes used to test metrics and identify important trends in productivity and performance

MG Performance



CRAY

NAS MG Linecounts

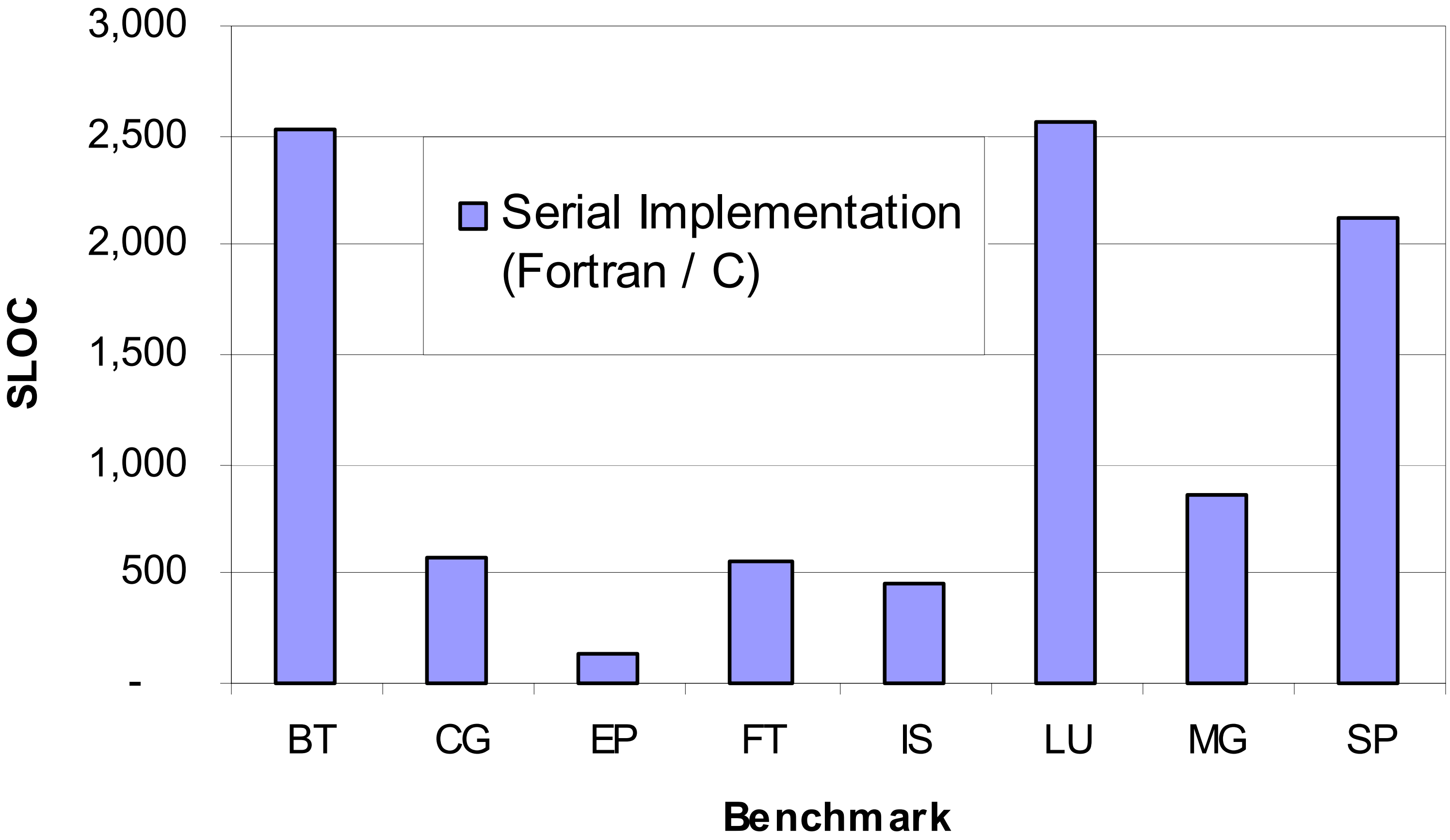


CRAY

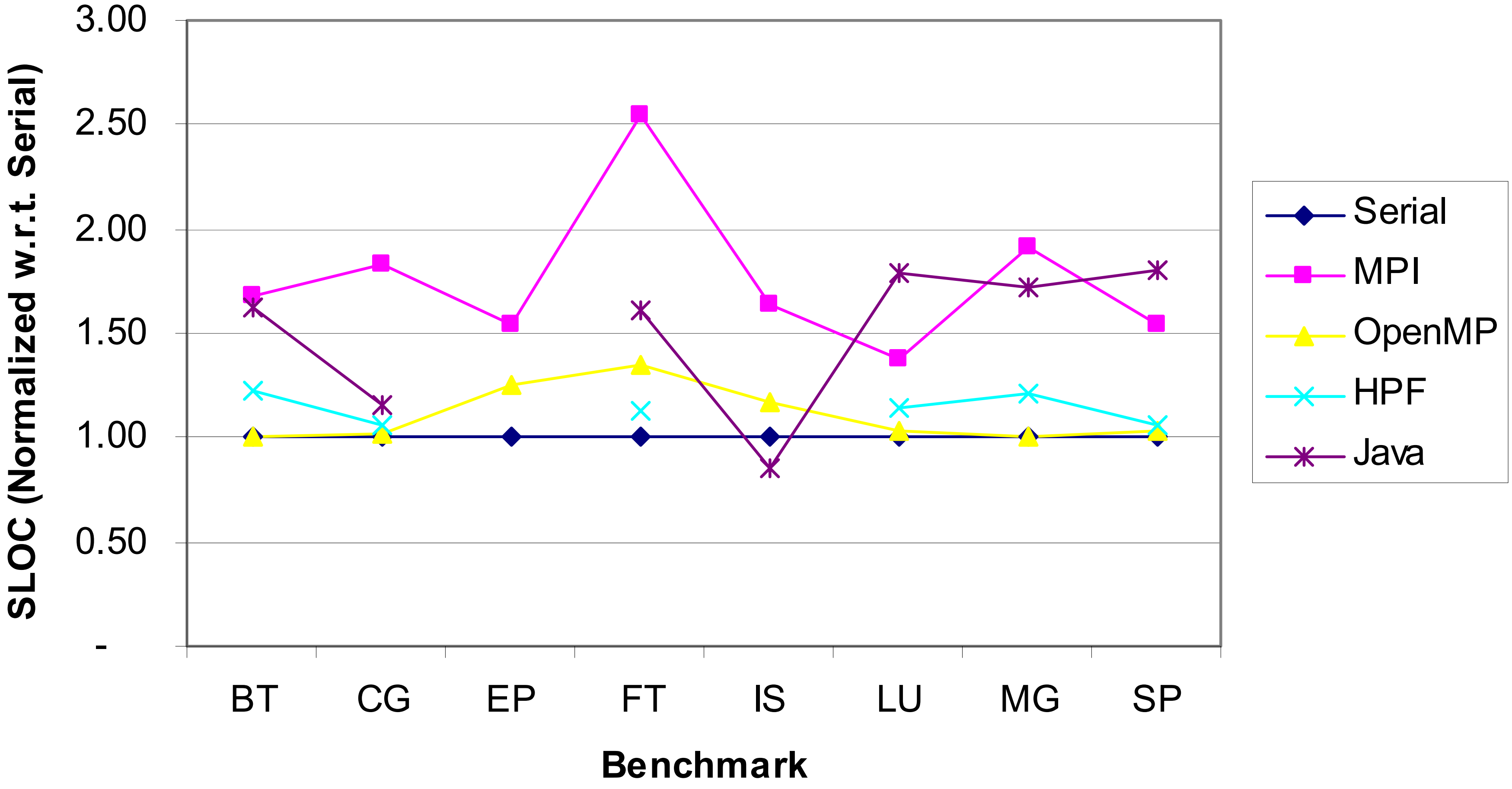
NPB Implementations

Benchmark	Languages							
	Serial Fortran	Serial C	Fortran / MPI	C / MPI	Fortan / OpenMP	C / OpenMP	HPF	Java
BT	🟩		🟩		🟩		🟩	🟩
CG	🟩		🟩		🟩		🟩	🟩
EP	🟩		🟩		🟩			
FT	🟩		🟩		🟩		🟩	🟩
IS		🟩		🟩		🟩		🟩
LU	🟩		🟩		🟩		🟩	🟩
MG	🟩		🟩		🟩		🟩	🟩
SP	🟩		🟩		🟩		🟩	🟩

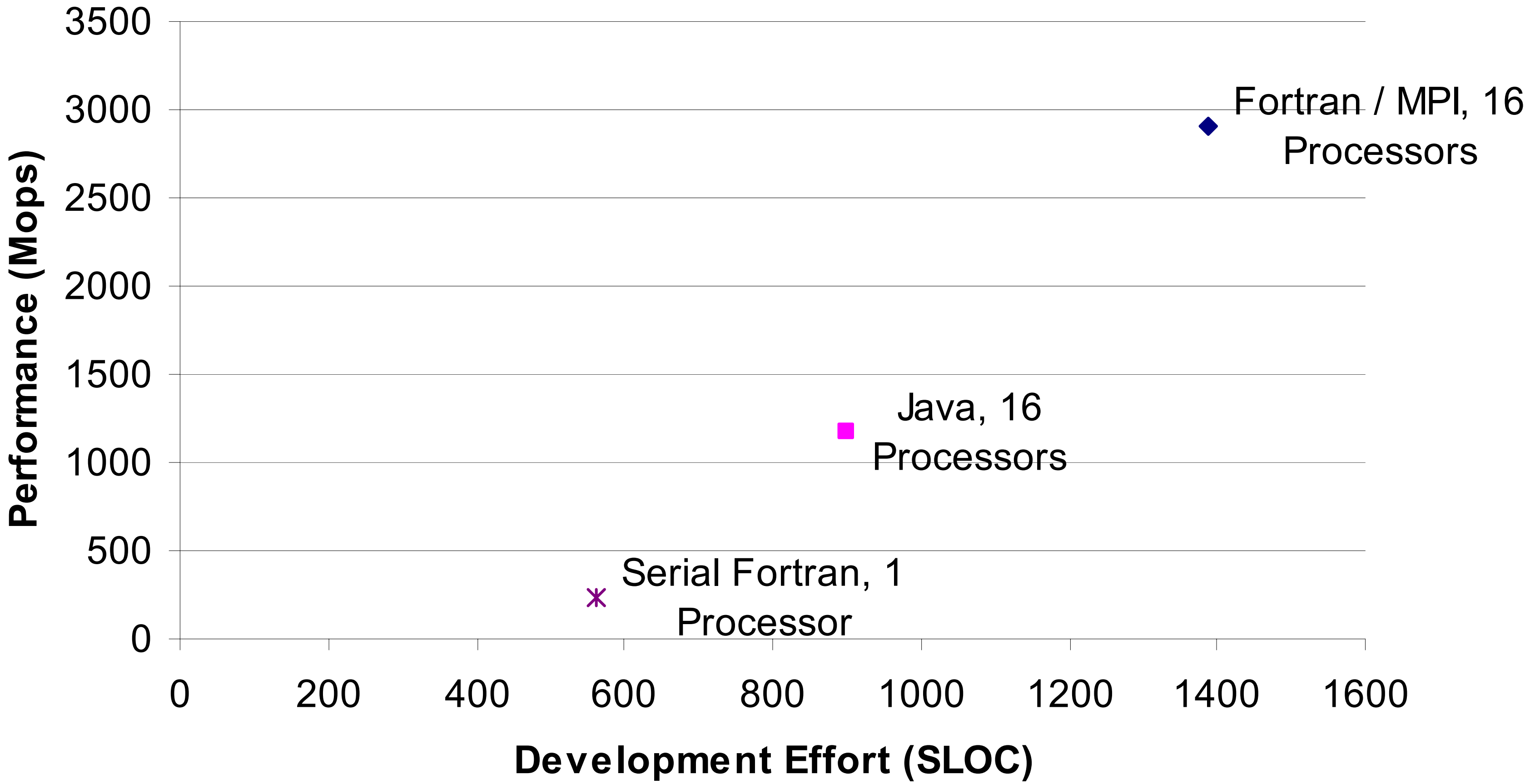
Source Lines of Code (SLOC) for the NAS Parallel Benchmarks (NPB)



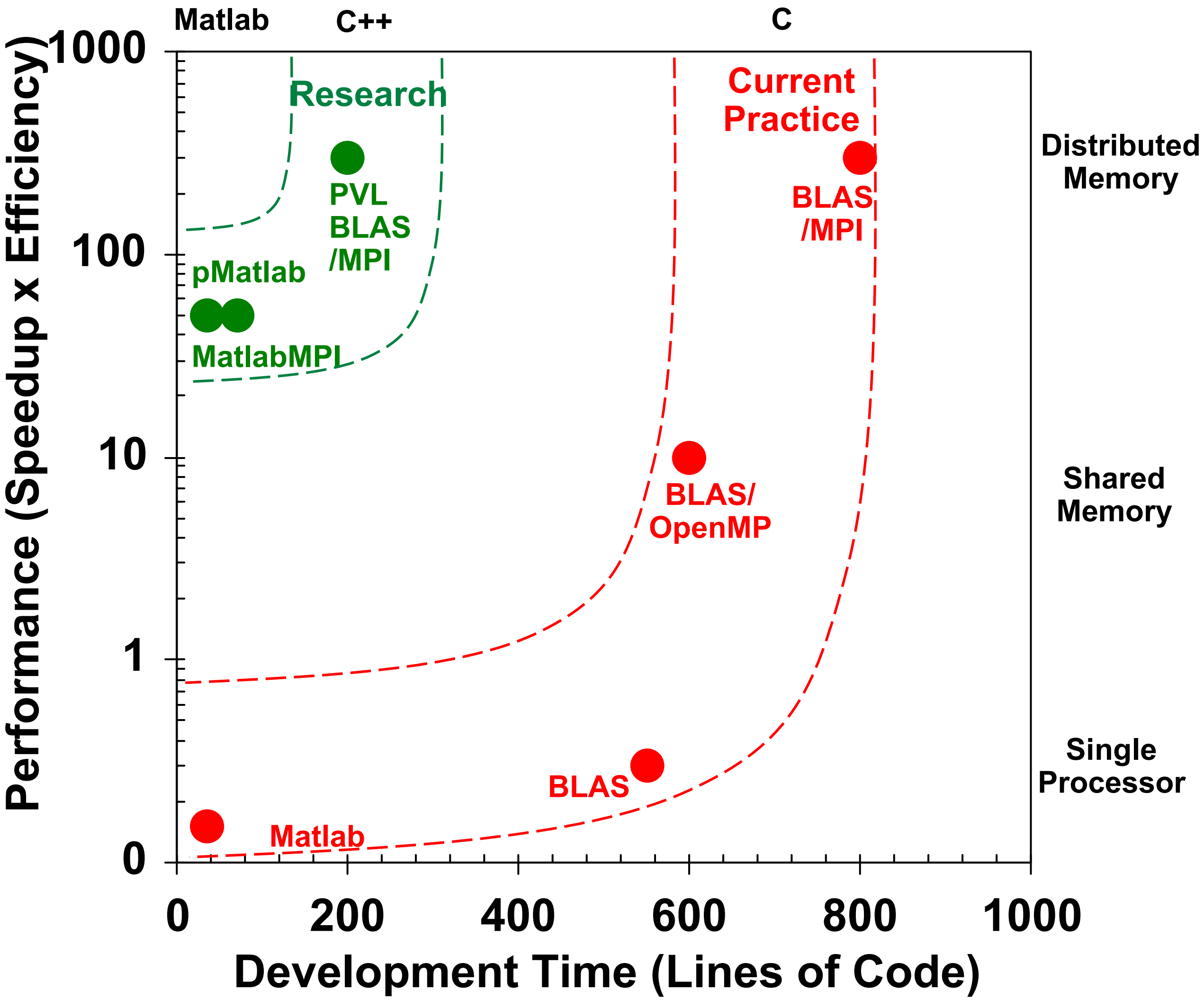
Normalized SLOC for All Implementations of the NPB



NAS FT Performance vs. SLOCs



Example Experiment Results (N=1)



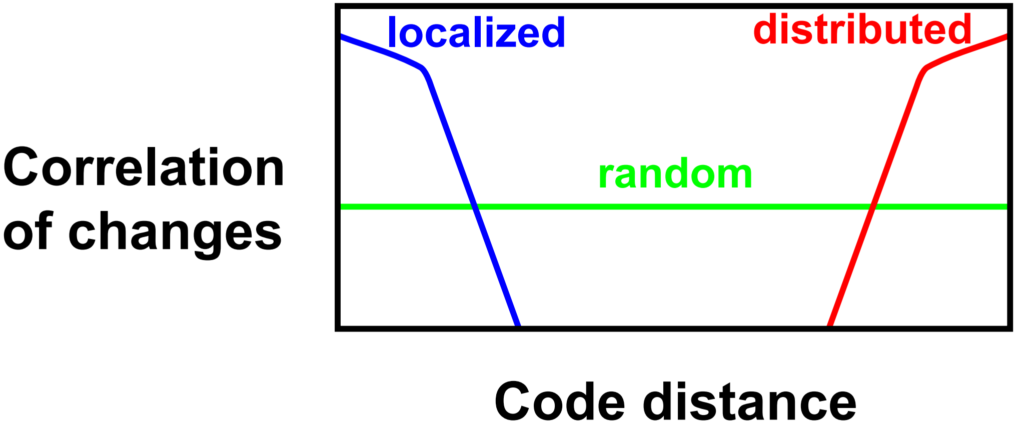
- Same application (image filtering)
- Same programmer
- Different langs/libs
  - •Matlab
  - •BLAS
  - •BLAS/OpenMP
  - •BLAS/MPI*
  - •PVL/BLAS/MPI*
  - •MatlabMPI
  - •pMatlab*

*Estimate

Controlled experiments can potentially measure the impact of different technologies and quantify development time and execution time tradeoffs

Novel Metrics

- HPC Software Development often involves changing code (Δx) to change performance (Δy)
  - 1st order size metrics measures scale of change E(Δx)
  - 2nd order metrics would measure nature of change $E(\Delta x^2)$
- Example: 2 Point Correlation Function
  - Looks at “distance” between code changes
  - Determines if changes are localized (good) or distributed (bad)



- Other Zany Metrics
  - See Cray talk

Outline

- Introduction
- Workflows
- Metrics
- **Models & Benchmarks**
  - ***Prototype Models***
  - ***A&P Benchmarks***
- Schedule and Summary

Prototype Productivity Models

Special Model with Work Estimator (Sterling)

$$\Psi_w = \frac{S_P \times E \times A}{c_f \times \left\{\Gamma \times \left(\bar{\rho} \bullet \bar{n}\right)\right\} + \left(c_m + c_o\right) \times T}$$

Utility (Snir)

$$\mathrm{P(S,A,U(.))} = \min_{\cos t} \frac{\mathrm{U(T(S,A,Cost))}}{\mathrm{Cost}}$$

Productivity Factor Based (Kepner)

$$\text{productivity}_{\substack{\text{GUPS}\\ \cdots \\ \text{Linpack}}} \approx \left(\frac{\left(\frac{\text{useful ops}}{\text{second}}\right)_{\substack{\text{GUPS}\\ \cdots \\ \text{Linpack}}}}{\text{Hardware Cost}}\right)\begin{pmatrix}\text{productivity}\\ \text{factor}\end{pmatrix}\begin{pmatrix}\text{mission}\\ \text{factor}\end{pmatrix}$$

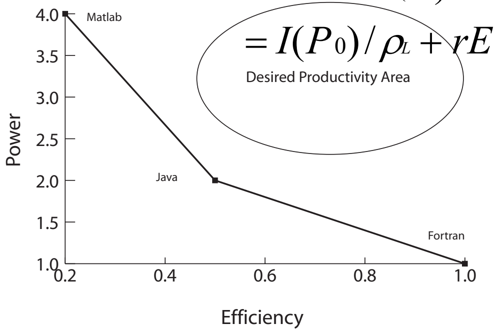
$$\begin{pmatrix}\text{productivity}\\ \text{factor}\end{pmatrix} \approx \begin{pmatrix}\text{Language}\\ \text{Level}\end{pmatrix} \times \begin{pmatrix}\text{Parallel}\\ \text{Model}\end{pmatrix} \times \text{Portability} \times \frac{\text{Availability}}{\text{Maintenance}}$$

Efficiency and Power (Kennedy, Koelbel, Schreiber)

$$T(P_L) = I(P_L) + rE(P_L)$$

$$= I(P_0) \cdot \frac{I(P_L)}{I(P_0)} + rE(P_0) \cdot \frac{E(P_L)}{E(P_0)}$$

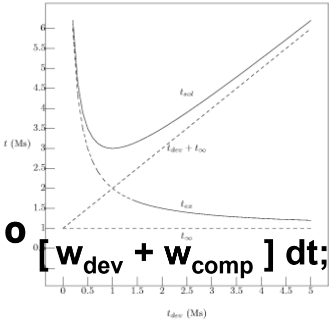
$$= I(P_0)/\rho_L + rE(P_0)/\varepsilon_L$$



CoCoMo II (software engineering community)

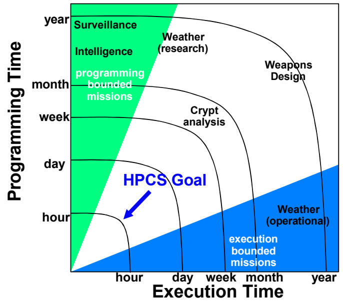
$$\begin{pmatrix}\text{Effort}\\ \text{Multipliers}\end{pmatrix} \mathbf{x}\ \mathrm{A}\ \mathbf{x} \left(\text{Size}\right)^{\left(\substack{\text{Scale}\\ \text{Factors}}\right)}$$

Least Action (Numrich)



$$S = {}^{\mathbf{o}}\,[\,w_{dev} + w_{comp}\,]\,dt; \qquad \delta S = 0$$

Time-To-Solution (Kogge)



HPCS has triggered ground breaking activity in understanding HPC productivity

-Community focused on *quantifiable* productivity (potential for broad impact)

-Numerous proposals provide a strong foundation for Phase 2

Code Size and Reuse Cost

Lines of code
Function Points
Reuse
Re-engineering
Maintenance

Code Size = (New) + (Reused) + (Re-engineered) + (Maintained)

Measured in lines of code or functions points (converted to lines of code)

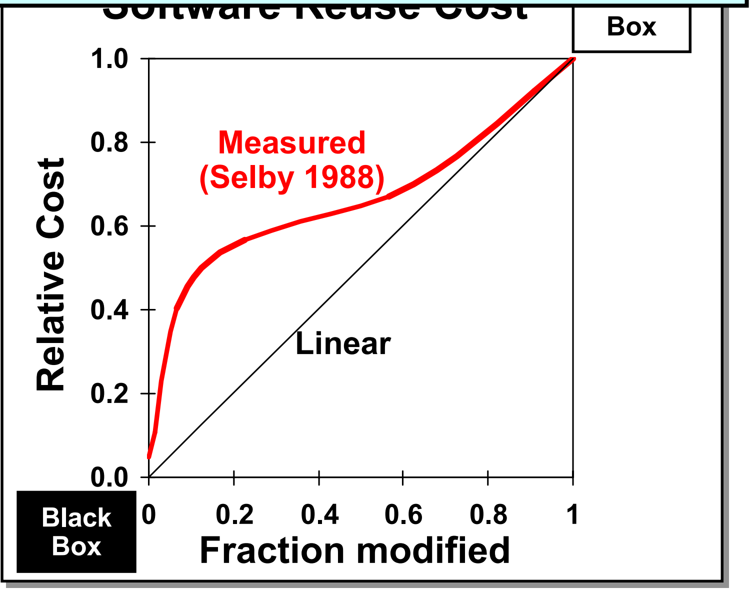
Lines per function point	
C, Fortran	~100
Fortran77	~100
C++	~30
Java	~30
Matlab	~10
Python	~10
Spreadsheet	~5

HPC Challenge Areas

Function Points
High productivity languages not available on HPC

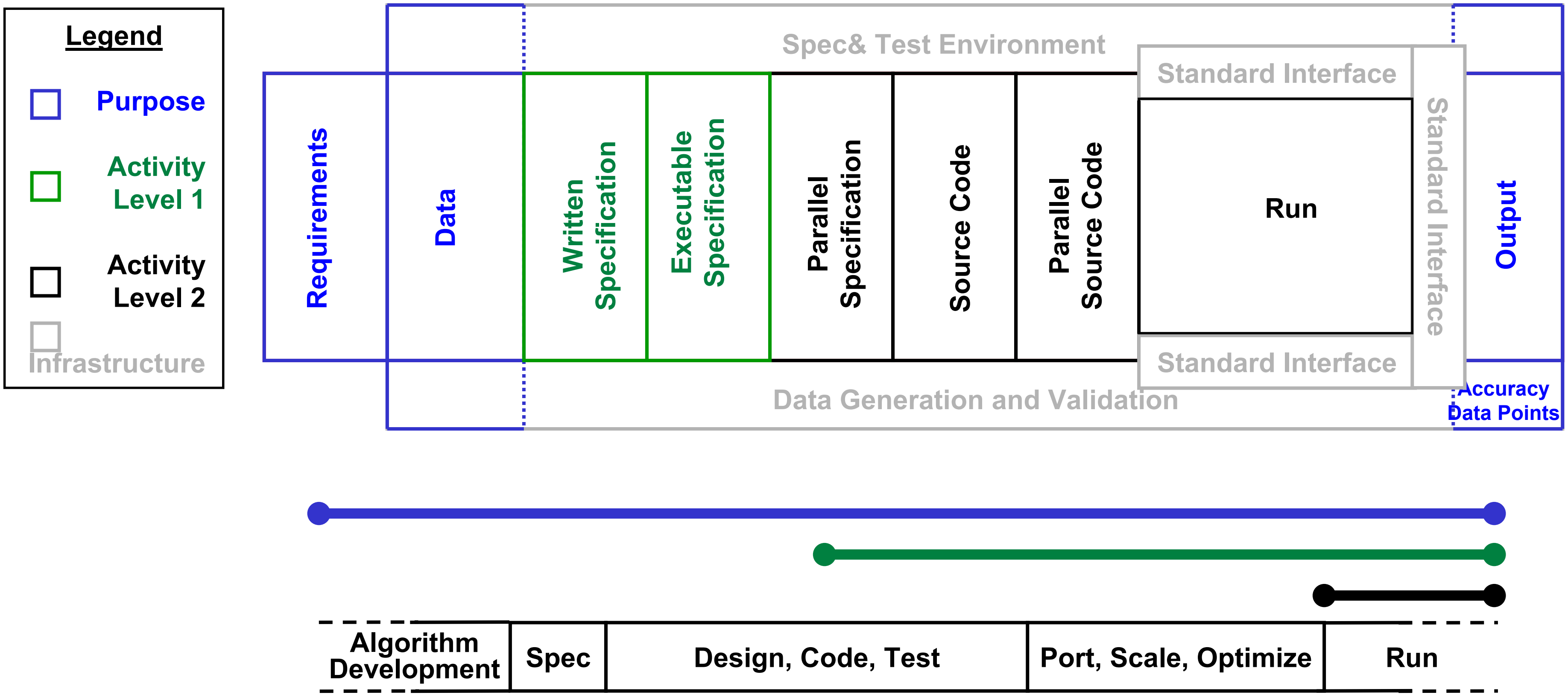
Reuse
Nonlinear reuse effects. Performance requirements dictate "white box" reuse model

- Code size is the most important software productivity parameter
- Non-HPC world reduces code size by
  - Higher level languages
  - Reuse
- HPC performance requirements currently limit the exploitation of these approaches



Activity & Purpose Benchmarks

Activity & Purpose Benchmark



Legend

□ Purpose

□ Activity Level 1

□ Activity Level 2

□ Infrastructure

Spec& Test Environment

Requirements

Data

Written Specification

Executable Specification

Parallel Specification

Source Code

Parallel Source Code

Standard Interface

Run

Standard Interface

Standard Interface

Output

Data Generation and Validation

Accuracy Data Points

Algorithm Development | Spec | Design, Code, Test | Port, Scale, Optimize | Run

Development Workflow

Activity Benchmarks define a set of instructions (i.e., source code) to be executed
Purpose Benchmarks define requirements, inputs and output
Together they address the entire development workflow

HPCS Phase 1 Example Kernels and Applications

Mission Area	Kernels	Application	Source
Stockpile Stewardship	Random Memory Access	UMT2000	ASCI Purple Benchmarks
	Unstructured Grids		
	Eulerian Hydrocode	SAGE3D	ASCI Purple Benchmarks
	Adaptive Mesh		
	Unstructured Finite Element Model	ALEGRA	Sandia National Labs
	Adaptive Mesh Refinement		
Operational Weather and Ocean Forecasting	Finite Difference Model	NLOM	DoD HPCMP TI-03
Army Future Combat Weapons Systems	Finite Difference Model	CTH	DoD HPCMP TI-03
	Adaptive Mesh Refinement		
Crashworthiness Simulations	Multiphysics Nonlinear Finite Element	LS-DYNA	Available to Vendors

Other Kernels	Lower / Upper Triangular Matrix Decomposition	LINPACK	Available on Web
	Conjugate Gradient Solver		DoD HPCMP TI-03
	QR Decomposition		Paper & Pencil for Kernels
	1D FFT		Paper & Pencil for Kernels
	2D FFT		Paper & Pencil for Kernels
	Table Toy (GUP/s)		Paper & Pencil for Kernels
	Multiple Precision Mathematics		Paper & Pencil for Kernels
	Dynamic Programming		Paper & Pencil for Kernels
	Matrix Transpose [Binary manipulation]		Paper & Pencil for Kernels
	Integer Sort [With large multiword key]		Paper & Pencil for Kernels
	Binary Equation Solution		Paper & Pencil for Kernels
	Graph Extraction (Breadth First) Search		Paper & Pencil for Kernels
	Sort a large set		Paper & Pencil for Kernels
	Construct a relationship graph based on proximity		Paper & Pencil for Kernels
	Various Convolutions		Paper & Pencil for Kernels
	Various Coordinate Transforms		Paper & Pencil for Kernels
	Various Block Data Transfers		Paper & Pencil for Kernels

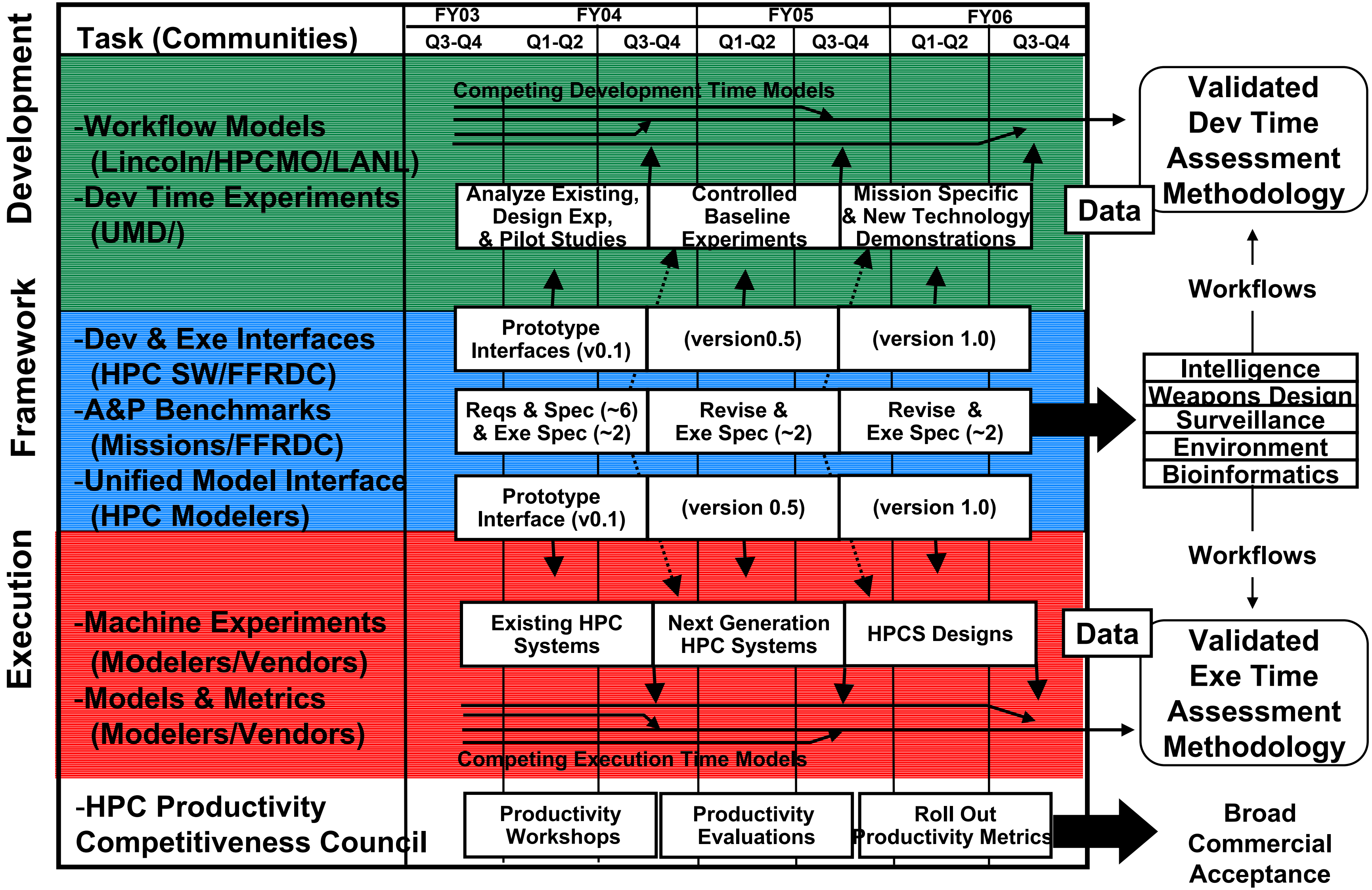
Bio-Application	Kernels	Application	Source
Quantum and Molecular Mechanics	Macromolecular Dynamics	CHARMM	http://yuri.harvard.edu/
	Energy Minimization		
	MonteCarlo Simulation		
Whole Genome Analysis	Sequence Comparison	Needleman-Wunsch	http://www.med.nyu.edu/rcr/rcr/course/sim-sw.html
		BLAST	http://www.ncbi.nlm.nih.gov/BLAST/
		FASTA	http://www.ebi.ac.uk/fasta33/
		HMMR	http://hmmer.wustl.edu/
Systems Biology	Functional Genomics	BioSpice (Arkin, 2001)	http://genomics.lbl.gov/~aparkin/Group/Codebase.html
	Biological Pathway Analysis		

Set of scope benchmarks representing Mission Partner and emerging Bio-Science high-end computing requirements

Outline

- Introduction
- Workflows
- Metrics
- Models & Benchmarks
- **Schedule and Summary**

Phase II Productivity Forum
Tasks and Schedule



Task (Communities)

FY03 FY04 FY05 FY06

Q3-Q4 Q1-Q2 Q3-Q4 Q1-Q2 Q3-Q4 Q1-Q2 Q3-Q4

Development

-Workflow Models (Lincoln/HPCMO/LANL)

-Dev Time Experiments (UMD/)

Competing Development Time Models

Analyze Existing, Design Exp, & Pilot Studies

Controlled Baseline Experiments

Mission Specific & New Technology Demonstrations

Framework

-Dev & Exe Interfaces (HPC SW/FFRDC)

Prototype Interfaces (v0.1)

(version0.5)

(version 1.0)

-A&P Benchmarks (Missions/FFRDC)

Reqs & Spec (~6) & Exe Spec (~2)

Revise & Exe Spec (~2)

Revise & Exe Spec (~2)

-Unified Model Interface (HPC Modelers)

Prototype Interface (v0.1)

(version 0.5)

(version 1.0)

Execution

-Machine Experiments (Modelers/Vendors)

Existing HPC Systems

Next Generation HPC Systems

HPCS Designs

-Models & Metrics (Modelers/Vendors)

Competing Execution Time Models

-HPC Productivity Competitiveness Council

Productivity Workshops

Productivity Evaluations

Roll Out Productivity Metrics

Validated Dev Time Assessment Methodology

Data

Workflows

Intelligence

Weapons Design

Surveillance

Environment

Bioinformatics

Workflows

Data

Validated Exe Time Assessment Methodology

Broad Commercial Acceptance

Summary

- Goal is to develop an acquisition quality framework for HPC systems that includes
  - Development time
  - Execution time

- Have assembled a team that will develop models, analyze existing HPC codes, develop tools and conduct HPC development time and execution time experiments

- Measures of success
  - Acceptance by users, vendors and acquisition community
  - Quantitatively explain HPC rules of thumb:

    "OpenMP is easier than MPI, but doesn't scale a high"

    "UPC/CAF is easier than OpenMP"

    "Matlab is easier the Fortran, but isn't as fast"
  - Predict impact of new technologies

Backup Slides

HPCS Phase II Teams

Industry:

IBM — PI: Elnozahy

Sun microsystems — PI: Gustafson

CRAY — PI: Smith

Goal:

- **Provide a new generation of economically viable high productivity computing systems for the national security and industrial user community (2007 – 2010)**

Productivity Team (Lincoln Lead)

MIT Lincoln Laboratory — PI: Kepner

ISI — PI: Lucas

University of Maryland — PI: Basili

UCSD — PI: Benson & Snavely

MITRE — PI: Koester

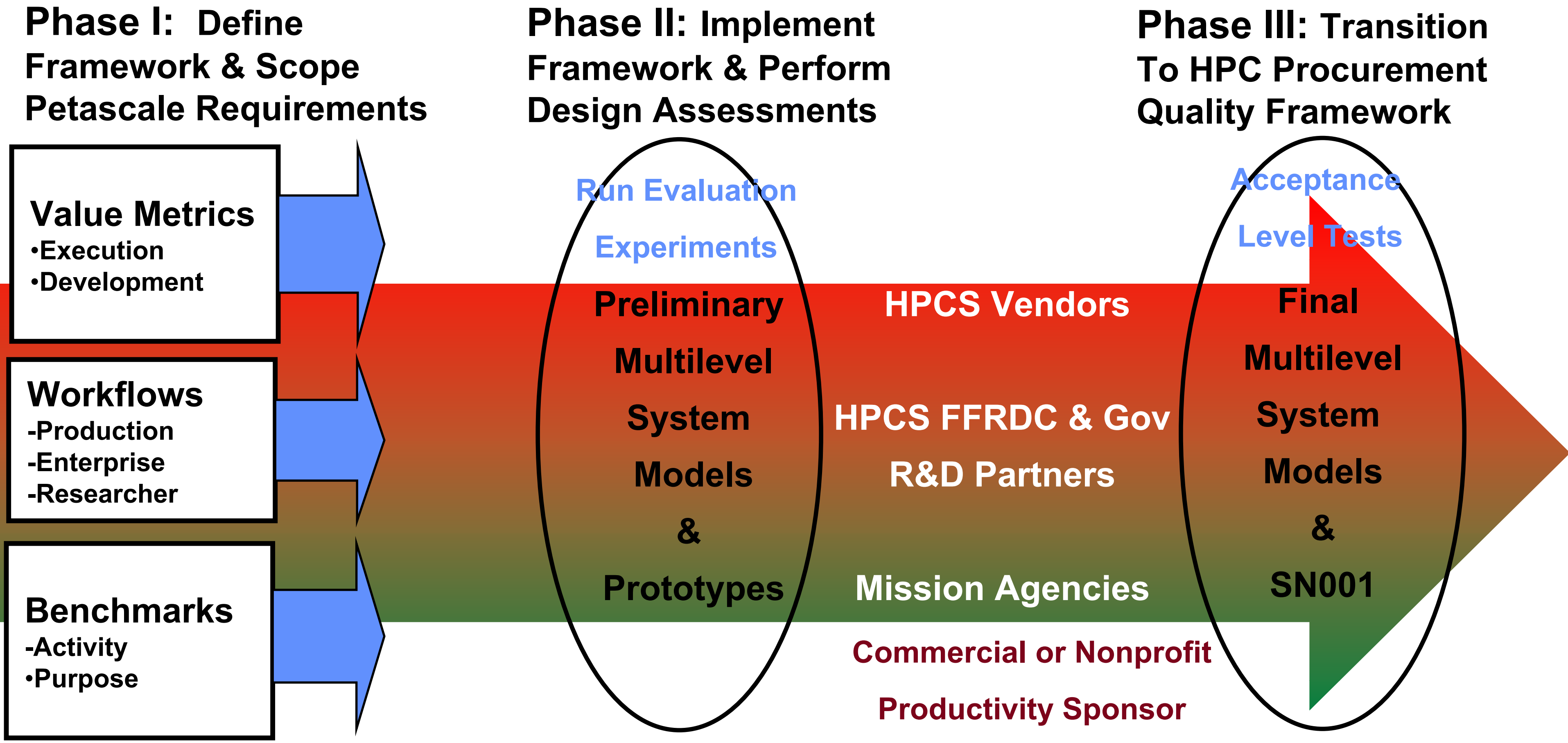
Los Alamos National Laboratory, ARGONNE, Berkeley Lab — PIs: Vetter, Lusk, Post, Bailey

UCSB, LCS, Ohio State, CodeSourcery — PIs: Gilbert, Edelman, Ahalt, Mitchell

Goal:

- **Develop a procurement quality assessment methodology that will be the basis of 2010+ HPC procurements**

Productivity Framework Overview



HPCS needs to develop a procurement quality assessment methodology that will be the basis of 2010+ HPC procurements